Pressurization Induced Structural Change of Titanium Phosphate Glass by X-ray and Neutron Total Scattering Analysis

Shi, Ying; Lönnroth, Nadja; Youngman, Randall E.; Smedskjær, Morten Mattrup

Publication date:
2017

Pressurization Induced Structural Change of Titanium Phosphate Glass by X-ray and Neutron Total Scattering Analysis

Ying Shi[1]*, Nadja Lonnroth[1], Randy Youngman[1], Morten M. Smedskjaer[2]

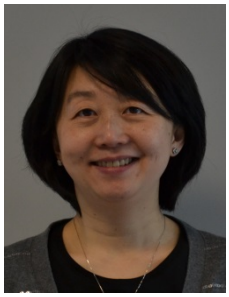
[1]Science and Technology Division, Corning Incorporated, Corning, NY14831,USA
[2]Department of Chemistry and Bioscience, Aalborg University, 9220 Aalborg, Denmark

ORAL Presentation

Abstract

Many experimental techniques probe glass structure at different length scales. Neutron and X-ray scattering are often the first choices since inter-atomic distances are provided by the real-space pair distribution function (PDF) which covers the whole interest range. Unfortunately direct and unambiguous interpretation of glass structure from PDFs is not possible due to severe peak overlap of different bonds. Instead, the differential PDF (DPDF) is often used to extract the partial PDF for more definite information.

In this study we used combined neutron and X-ray total scattering analysis to study the structural change of titanium phosphate $0.73TiO2{\cdot}0.27P_2O_5$ glass induced by 1GPa pressurization performed at glass transition temperature. Because titanium has negative scattering length by neutron scattering and positive weighting factor by X-ray scattering, a Ti-containing glass is a perfect candidate for combined X-ray and neutron differential scattering analysis to extract the individual P-O and Ti-O pair distributions. The individual partial Ti-O and P-O bond distribution function (noted as nDFs) were extracted from combined neutron and X-ray data. The differential PDF technique was applied again, by subtracting the as-made partial nDF from their corresponging pressurized partial nDF. It will be shown by differential PDF analysis that the D-$n_{Ti\text{-}O}$DF has a negative peak at 1.80Å and a positive peak at 2.10Å. By comparing to a crystal structure related to the glass composition$Ti_5O_4(PO_4)_4$, the shorter Ti-O bond length correponds to bonds in the TiO_6 octahedra which are corner shared with other TiO_6 octahedra, the longer bonds correspond to Ti-O bonds which are face shared by two TiO_6 octahedra. In conlcusion, a 2mol% corner sharing to face sharing transition of titanium octahedra seems to be the main cause of density increase by pressurization as defined by the utilized techniques.



Ying Shi is Sr. Research Scientist of Characterization Science Division of Corning Incorporated. She received her Ph.D. in Condensed Matter Physics from Institute of Physics, Chinese Academy of Science in 1997. Before joining Corning in 2011, she held two post-doctor positions and two industrial positions, all of those involved structure characterization of crystalline materials. Since 2013, she started exploring total scattering analysis to study glass structure, using both neutron and synchrotron X-ray.